

CLAIMS

1. A method of analyzing sequences of atomic groups including a first sequence having m atomic groups and a second sequence having n atomic groups where m and n are integers, comprising the steps of:
- a) preparing an array S[i] having array elements S[0] to S[m];
  - b) initializing all array elements of the array S[i] to zero and initializing an integer j to 1;
  - c) adding 1 to each array element S[i] that is equal to an array element S[r] and that  $i \geq r$  if the array element S[r] is equal to an array element S[r-1] where r is an occurrence position of j-th atomic group of the second sequence in the first sequence;
  - d) adding 1 to the integer j;
  - e) repeating the step c) and d) until the integer j exceeds n; and
  - f) obtaining a longest common atomic group number between the first and the second sequences from a value of the array element S[m].
2. A method of claim 1, further comprising the steps of:
- g) preparing an array data[k] having array elements data[0], data[1] ...;
  - h) storing paired data (r, j) in an array element data[k] if the array element S[i] is changed in the step c) where  $k = S[r]$ ;
  - i) linking the paired data (r, j) stored in the step h) to paired data (r', j') if  $r' < r$  and  $j' < j$  where the paired data (r', j') is one stored in an array element data[k-1]; and
  - j) obtaining a longest common subsequence between the first and the second sequences and occurrence positions of the longest common subsequence in the first and the second sequence by tracing the link formed in the step i).

3. A method of claim 1 further comprising the step of

k) evaluating homology between the first and the second sequences based on the longest common atomic group number and a value of one of m and n.

4. A method of claim 3, further comprising the step of

1) searching for a sequence that is homologous with the first sequence from among a plurality of sequences, by successively assigning one of the plurality of sequences to the second sequence and executing the steps a) to f) and k).

5. A method of analyzing three-dimensional structures including a first structure expressed by three-dimensional coordinates of elements belonging to a first point set and a second structure expressed by three-dimensional coordinates of elements belonging to a second point set, comprising the steps of:

a) generating a combination of correspondence satisfying a restriction condition between the elements belonging to the first point set and the elements belonging to the second point set from among all candidates for the combination of correspondence; and

b) calculating a root means square distance between the elements corresponding in the combination of correspondence generated in the step a).

6. A method of claim 5, wherein the restriction condition includes order relation of the elements in the first and the second point sets that are ordered.

7. A method of claim 5, wherein the restriction condition includes proximity in a geometric relationship among a plurality of elements close to each other.

8. A method of claim 6 wherein the restriction condition includes proximity in a geometric relationship among a plurality of elements close to

each other.

9. A method of claim 5, wherein the restriction condition includes a condition such that a candidate for the combination of correspondence satisfies a threshold value condition.

10. A method of claim 6, wherein the restriction condition includes a condition such that a candidate for the combination of correspondence satisfies a threshold value condition.

11. A method of claim 5, wherein the restriction condition includes a condition such that an attribute value of each of the elements belonging to the first point set coincides with an attribute value of the corresponding element belonging to the second point set in a candidate for the combination of correspondence.

12. A method of claim 6, wherein the restriction condition includes a condition such that an attribute value of each of the elements belonging to the first point set coincides with an attribute value of the corresponding element belonging to the second point set in a candidate for combination of correspondence.

13. A method of analyzing three-dimensional structures including a first structure expressed by three-dimensional coordinates of elements belonging to a first point set and a second structure expressed by three-dimensional coordinates of elements belonging to a second point set, comprising the steps of:

a) dividing the second point set into a plurality of subsets having a size that is determined by the size of the first point set;

b) generating a combination of correspondence satisfying a restriction condition between the elements belonging to the first point set and the elements belonging to each of the subsets of the second point set from among all candidates for the combination of correspondence; and

c) calculating a root mean square distance between the elements corresponding in the combination of correspondence generated in the step b).

5 14. A method of claim 13, wherein the second point set is divided into the subsets so that the number of elements belonging to each of the subsets is a function of the number of elements belonging to the first point set.

10 15. A method of claim 13, wherein the second point set is divided into the subsets so that a spatial size of each of the subsets is nearly equal to a spatial size of the first point set.

16. A method of analyzing three-dimensional structures including a first structure expressed by  
15 three-dimensional coordinates of elements belonging to a first point set and a second structure expressed by three-dimensional coordinates of elements belonging to a second point set, comprising the steps of:

20 a) dividing the first point set and second point set into first subsets and second subsets, respectively, according to a secondary structure exhibited by the three-dimensional coordinates of the elements of the first and the second point sets;

25 b) generating a combination of correspondence satisfying a first restriction condition between the first subsets and the second subsets from among candidates for the combination of correspondence;

30 c) determining an optimum correspondence between the elements belonging to each pair of subsets corresponding in the combination of correspondence generated in the step b), and

35 d) calculating a root mean square distance between all of the elements corresponding in the optimum correspondence in the step c).

17. A method of claim 16, wherein the optimum correspondence determining step comprising the

00910054 072001

substeps of:

i) generating a combination of correspondence satisfying a second restriction condition between the elements belonging to the subsets corresponding in the combination of the correspondence generated in the step b);

ii) calculating a root mean square distance between the elements corresponding in the combination of the correspondence generated in the substep i);

iii) selecting a combination of the correspondence as the optimum correspondence according to the value of the root mean square distance value calculated in the substep ii).

18. An apparatus for analyzing sequences of atomic groups including a first sequence having m atomic groups and a second sequence having n atomic groups where m and n are integers, comprising:

means for preparing an array S[i] having array elements S[0] to S[m];

means for initializing all array elements of the array S[i] to zero and initializing an integer j to 1;

means for renewing the array S[i] by adding 1 to each array element S[i] that is equal to an array element S[r] and that  $i \geq r$  if the array element S[r] is equal to an array element S[r-1] where r is an occurrence position of j-th atomic group of the second sequence in the first sequence;

means for incrementing the integer j by 1;

means for repeatedly activating the renewing means and the incrementing means until the integer j exceeds n; and

means for obtaining a longest common atomic group number between the first and the second sequences from a value of the array element S[m].

19. An apparatus of claim 18, further comprising:

means for preparing an array data[k]  
having array elements data[0], data[1]...;

means for storing paired data (r, j) in  
an array element data [k] if the array element S[i] is  
5 changed by the renewing means where  $k = S[r]$ ;

means for linking the paired data (r, j)  
stored by the storing means to paired data (r', j') if  
 $r' < r$  and  $j' < j$  where the paired data (r', j') is  
one stored in an array element data [k-1]; and

- 10 means for obtaining a longest common  
subsequence between the first and the second sequences  
and occurrence positions of the longest common  
subsequence in the first and the second sequence by  
tracing the link formed by the linking means.

15 20. An apparatus of claim 18, further comprising  
means for evaluating homology between  
the first and the second sequences based on the  
longest common atomic group number and a value of one  
of m and n.

20 21. An apparatus for analyzing three-dimensional  
structures including a first structure expressed by  
three-dimensional coordinates of elements belonging to  
a first point set and a second structure expressed by  
three-dimensional coordinates of elements belonging to  
25 a second point set, comprising:

means for generating a combination of  
correspondence satisfying a restriction condition  
between the elements belonging to the first point set  
and the elements belonging to the second point set  
30 from among all candidates for the combination of  
correspondence; and

means for calculating a root mean square  
distance between the elements corresponding in the  
combination of correspondence generated by the  
35 generating means.

22. An apparatus for analyzing three-dimensional  
structures including a first structure expressed by

three-dimensional coordinates of elements belonging to a first point set and a second structure expressed by three-dimensional coordinates of elements belonging to a second point set, comprising the steps of:

- 5 means for dividing the second point set into a plurality of subsets having a size that is determined by the size of the first point set;
- means for generating a combination of correspondence satisfying a restriction condition
- 10 between the elements belonging to the first point set and the elements belonging to each of the subsets of the second point set from among all candidates for the combination of correspondence; and
- means for calculating a root mean square
- 15 distance between the elements corresponding in the combination of correspondence generated by the generating means.

23. An apparatus for analyzing three-dimensional structures including a first structure expressed by three-dimensional coordinates of elements belonging to a first point set and a second structure expressed by three-dimensional coordinates of elements belonging to a second point set, comprising:

- means for dividing the first point set
- 25 and the second point set into first subsets and second subsets, respectively, according to a secondary structure exhibited by the three-dimensional coordinates of the elements of the first and the second point sets;
- 30 means for generating a combination of correspondence satisfying a first restriction condition between the first subsets and the second subsets from among candidates for the combination of correspondence;
- 35 means for determining an optimum correspondence between the elements belonging to each pair of subsets corresponding in the combination of

correspondence generated in the generating means, and means for calculating a root mean square distance between all of the elements corresponding in the optimum correspondence.

5

00010001, 072301